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NEWS 23 MAR 06 INFADOCDB and INPAFAMDB enhanced with new display formats

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3.

AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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STRUCTURE FILE UPDATES: 6 MAR 2009 HIGHEST RN 1116745-20-0
DICTIONARY FILE UPDATES: 6 MAR 2009 HIGHEST RN 1116745-20-0

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<http://www.cas.org/support/stnqgen/stndoc/properties.html>

=>
Uploading C:\Program Files\STNEXP\Queries\10526507\formula I 3_8_09.str



chain nodes :
 8 9 10 11 12 13 15 22
 ring nodes :
 1 2 3 4 5 6 16 17 18 19 20
 chain bonds :
 5-8 8-9 9-10 10-11 11-12 11-13 12-15
 ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-20 17-18 18-19 19-20
 exact/norm bonds :
 5-8 8-9 9-10 10-11 11-12 11-13 12-15 16-17 16-20 17-18 18-19 19-20
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
 isolated ring systems :
 containing 1 : 16 :

G1:H,Cb,Ak
 G2:O,S

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS
 11:CLASS 12:CLASS 13:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
 22:Atom 23:Atom

Generic attributes :
 22:
 Saturation : Unsaturated

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 H, C₆, Ak
G2 O, S

Structure attributes must be viewed using STN Express query preparation.

=> s 11
SAMPLE SEARCH INITIATED 17:14:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 35989 TO ITERATE

5.6% PROCESSED 2000 ITERATIONS	0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)	
SEARCH TIME: 00.00.01	

FULL FILE PROJECTIONS:	ONLINE **COMPLETE**	
	BATCH **COMPLETE**	
PROJECTED ITERATIONS:	708437 TO 731123	
PROJECTED ANSWERS:	0 TO 0	

L2 0 SEA SSS SAM L1

=> s 11 full
FULL SEARCH INITIATED 17:15:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 720424 TO ITERATE

90.3% PROCESSED 650410 ITERATIONS	24 ANSWERS
96.2% PROCESSED 693179 ITERATIONS	24 ANSWERS
100.0% PROCESSED 720424 ITERATIONS	24 ANSWERS
SEARCH TIME: 00.00.40	

L3 24 SEA SSS FUL L1

=> fil caplus	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	187.32	187.98

FILE 'CAPLUS' ENTERED AT 17:15:47 ON 08 MAR 2009
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FILE COVERS 1907 - 8 Mar 2009 VOL 150 ISS 11
FILE LAST UPDATED: 6 Mar 2009 (20090306/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s 13
L4          15 L3
=> d ibib 1-5
```


14 ANSWER 6 OF 15 CAPTION COPYRIGHT 2009 ACS on 9/7/09 (Continued)
X = CO₂(CH₂)_n, each N-(un)substituted CONH(CH₂)_n or NHCO(CH₂)_n (wherein n

ng to g, to give, after distillation of the solvent and silica gel chromatog., 723 mg of 4-[4-(trifluoromethyl)-1-*l*-biphenyl-2-ylmethyl]aniline; trifluoromethyl acid was added to the residue, and the product was isolated by column chromatog. (silica gel, 11 % *N*-Mei) and the triglyceride transport between lipoproteins by MTR was determined with CDS of 0.65 and 0.39 mm, resp., and the separation of apolipoprotein B with HPLC.

In a final step, HMGCoA with CDS of 0.65 and 0.46, resp., Pharmaceutical fractionation was performed with a column packed with SiO_2 (Merck), eluted with $\text{CH}_2\text{Cl}_2\text{-}(\text{4}-\text{trifluoromethyl)-1-l-biphenyl-2-ylmethyl})\text{aniline}\text{-}[\text{J}-\text{Gly}]$ and $\text{CH}_2\text{Cl}_2\text{-}(\text{4}-\text{trifluoromethyl)-1-l-biphenyl-2-ylmethyl})\text{phenylmethane acid di-Et est}$. The fractions were collected and the product was isolated by column chromatog. (silica gel, 20 % *N*-Mei). The product was characterized by IR, $^1\text{H-NMR}$, $^{13}\text{C-NMR}$ (chemical shift), $^{19}\text{F-NMR}$ (trifluoromethyl resonance), MS (molecular fragmentation), TIR

[*Preparation*] $\text{Pf}^{\text{a}}\text{Km}^{\text{b}}\text{Bm}^{\text{c}}\text{Th}^{\text{d}}\text{Bz}^{\text{e}}$ (*Pharmaceutical activity*) [*BMP*] (*Biological preparation*); *TBS* [*Therapeutic use*]; *EDCL* (*Biological study*); *PREP* (*Preparation*); *USSS* [*Cass*].
[preparation of [1-hexenyl]carboxylic acid esters as microsomal triglyceride transfer protein (MTP) inhibitors for treatment or prevention of diseases]
 55441-10-0
[Propendipine acid, 2-phenyl-2-[4-(2-[3-methoxybenzyl]benzoyl)amino]phenyl]acetyl oxime]methyl-, 1,3-diethyl ester [CA

INDEX NAME)

$$\text{Ph} \xrightarrow{\text{O}} \text{Ph} \xrightarrow{\text{O}}$$

$$\text{CH}_2=\text{CH}-\text{CH}_2-\text{C}(=\text{O})-\text{O}-\text{CH}_2-\text{C}(=\text{O})-\text{O}-\text{CH}_2-$$

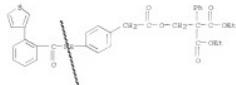
The diagram shows two chemical structures side-by-side. On the left is 4-phenyl-1-butene, which consists of a four-carbon chain with a double bond between the first and second carbons, and a phenyl group attached to the fourth carbon. On the right is 4-phenyl-1-butene-3-one, which has the same four-carbon chain with a double bond between the first and second carbons, but it also features a carbonyl group (a carbon double-bonded to an oxygen atom) attached to the third carbon.

$$\text{C}_6\text{H}_5\text{CH}_2\text{C}(\text{OEt})_2 \rightleftharpoons \text{C}_6\text{H}_5\text{CH}_2\text{COEt} + \text{Et}_2\text{O}$$

The reaction scheme illustrates the formation of 2-phenyl-4-oxo-4H-1,3-dioxin-5-carboxylic acid. It begins with the reaction of phenylmagnesium bromide ($\text{C}_6\text{H}_5\text{MgBr}$) with 2,3-dihydro-1,3-dioxin-5-carboxylic acid ($\text{C}_4\text{H}_6\text{O}_3$). The product is 2-phenyl-4-oxo-4H-1,3-dioxin-5-carboxylic acid ($\text{C}_9\text{H}_8\text{O}_4$).

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Searched by J



LA ANSWER 9 OF 15 CAPTION COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 199153441 CAPTION

DOCUMENT NUMBER: 1902621459

TITLE: A Quantitative Quantitative Structure-Activity Relationship of Interleukin-1 β Converting Enzyme Inhibitors: A Comparative Molecular Field Analysis Study

AUTHOR(S): Kulkarni, Sastha S.; Kulkarni, Vilas H.

CORPORATE SOURCE(S): Department of Chemical Technology Pharmaceutical Division, University of Mumbai, Mumbai, 400 093, India

SOCPACs: JOURNAL OF MEDICAL CHEMISTRY (1999), 42(7), 373-380
CROSSREFS: 199153441-199153441-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Cited reference

LANGUAGE: English

AB: A three-dimensional quantitative structure-activity relationship (QSAR) study was performed to predict the biological activity of a series of interleukin-1 β converting enzyme (ICE) inhibitors. The compounds studied have been reported to be time-dependent inhibitors of ICE.

This study was performed using 49 compounds, in which the CoMFA models were developed using a training set of 39 compounds. All the compounds were noted using the X-ray crystal structure of tetrapeptide aldehyde inhibitor/ICE (TAPI). The remaining 10 compounds were considered as test set compounds and as P2 phosphotyrosine isozyme. Superimposition were performed using two alignment rules, namely, an alignment of the structures based on

MMO fitting of the backbone heavy atoms of each structure to compound 2 and an alignment based on SYBYL QSAR rigid body field fit of the steric and electrostatic fields of the molecule to the fields of compound 2. Use of LOMO energies or CleopP as added descriptors in the QSAR table did not improve the significance of the CoMFA models. Steric and electrostatic fields of the molecules were used to predict the biological activity of the ICE structure-activity relationships. The predictive ability of the CoMFA model was evaluated by using a test set of 10 compounds, i.e., peptide 2 (aligned to 2),. Further comparison of the coefficient contour maps with the steric and

electrostatic properties of the receptor show a high level of agreement. (J. Med. Chem. 1999, 42, 373-380)

IT 173025-42-4

RL: AAC (Biological activity or effect, except adverse); RRU

BIOLOGICAL ACTIVITY: (BIO): (Biological activity or effect, except adverse); (BIO)

(QSAR of interleukin-1 β converting enzyme inhibitors: comparative

mol. field anal. study)

JH 199153441-199153441-199153441-2623

CH Benzoic acid, 2,6-dichloro-, (3S)-4-carboxy-2-oxo-3-[(6-oxo-5-

[(2-phenylmethyl)carbonyl]amino]-2-[2-(2-methoxy-1-phenyl-

pyrimidinyl)acetyl] ester (SCE) (CA INDEX NAME)

LA ANSWER 10 OF 15 CAPTION COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1991534190 CAPTION

DOCUMENT NUMBER: 1902621459

ORIGINAL REFERENCE NO.: 1274602154, 12018a

TITLE: Preparation of N-(6-oxo-1-pyrimidinylacetyl)aspartic acid analogs as interleukin-1 β -converting enzyme inhibitors

INVENTOR(S): Nolte, Roland E.; Prouty, Catherine F.; Chetverudova, Paulina; Schmid, Stanley F.

PATENT ASSIGNEE(S): Sanofi, Fr.

SOURCE(S): U.S. Pat. 5,211,329, filed -18-part in part of U.S. Ser. No. 221,712, filed 12/29/88, issued 6/9/93

PATENT NUMBER: 5,211,329

ISSUED DATE: 1993-06-09

FAMILY ACC. INDN. COUNT: 2

PATENT INFORMATION:

PATENT NO.: US 5470454

KIND: PCT

DATE: 19970923

APPLICATION NO.: 1995-559970

DATE: 19951210

US 1145292

A

DATE: 19970507

US 1995-193258

A

DATE: 19951210

US 1145293

A

DATE: 19970507

US 1995-193259

A

DATE: 19970507

US 1145287

T

DATE: 20040331

PT 1995-915448

A

DATE: 20040416

CH 1154462

A

DATE: 20040416

US 6128200

A

DATE: 20000119

US 2001003750

A3

DATE: 20000114

US 6143768

B2

DATE: 20000818

US 1995-221702

B2

DATE: 19960915

US 1995-559870

A1

DATE: 19951210

US 1997-877380

A3

DATE: 2000740623

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US 1995-559870

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DATE: 19960915

US 1997-877380

A3

DATE: 19970617

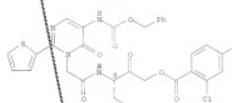
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A3

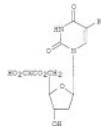
DATE

(Cont'd next)

2013-01-01



- 14 ANSWER 12 OF 15 CAPUS COPYRIGHT 2009 ACM on STM
ANSWER NUMBER: 1998122812 CAPUS
DOCUMENT NUMBER: 12512
REFERENCE NUMBER: 10464234,6644
TITLE: Synthesis of nitriles to thiadiazine and thiazine substituted triphosphates
AUTHOR(S): Walmar, Ulf; Norrby, Anna-Brittta; Gronowitz, Baloo; Johansson, Niia Gunnar
CORPORATE SOURCE: Department of Biotechnology, Royal Institute of Technology, Lund, S-223
SOURCE: Nucleic Acids & Nucleotides (1996), 15(15), 1059-1076
PUBLISHER: Dekker
JOURNAL TITLE: Journal
LANGUAGE: English



- A8 Dibenzylidene acetal 5'-monooesters of Uracilidine and 2-(2-thienyl)-2'-deoxyuridine 1' N = 2-thienyl X = (CH₂)₂; 1,4-phenyleneoxydiphenyl n = 3-5 have been synthesized and evaluated as triple-stranded DNA binders. The compounds adopt different conformations fixing the triphosphate group at different positions. The one having overall best inhibitory activities against HSV-1 and HSV-2 is 1' N = 2-thienyl X = (CH₂)₂ [KCI (IC₅₀) = 4 μM].

177779-39-39 177779-39-39 177779-40-79
 KI RCT (Reagent); BHP (Synthetic preparation); PMPF (Preparation; KACT (Reagent or reagent))
 (positive) and virucidal activity of uridine and thiacytosine/uridine monooesters of alkylendiaminopyrimidines

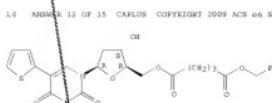
177779-39-39 CUSO₄
 Cu²⁺ 177779-39-39 (2-thienyl)-, 5'-{[phenylmethyl] pentamethiodioate} (KCI)
 [CIA: INDEX: NAME]

Absolute stereochemistry:

Absolute Strengths

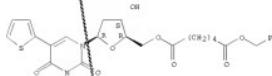
L4 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2009 JCS on 5TH

(Continued)



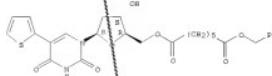
- NN 17779-3-4 CAPLUS
 CM Uridine, 2'-deoxy-5-(2-thienyl)-, 5'-(phenylmethyl hexanedioate) (PCP)
 (a.k.a. UTP)

Absolute stereochemistry



- BN 177779-40-7 CAPLUS
CN Uridine, 2'-deoxy-5'-(2-thienyl)-, 5'-(phenylmethyl heptanedioate) (PGL
(CA INDEX NAME))

Absolute stereochemistry



LA ANSWER IS OF 15 CAPTION COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 1970-31599 CARBON

DOCUMENT NUMBER: 721-1599

ORIGINAL REFERENCE NO.: 721-1599-577a

TITLE: Antiinflammatory Esters and Thioesters

INVENTOR(S): O'Meara, Derrick M.

PUBLICATION ASSIGNEE(S): 2000, Ethical Chemical Industries Ltd.

SOCIAL SECURITY: Gen. Office, 44 pp.

COUNTRY CODE: GB/GBR/GB

DOCUMENT TYPE: PCT/INTL

LANGUAGE: German

FAMILY ACC.: 20M, COUNT: 2

PRIZE UNDERRATING:

PAIDIN ID:	KIND	DATE	APPLICATION NO.	DATE
LA 2929301	A	1969-0223	DE 1969-1919801	19690416
LA 2929302	A	1969-0223	DE 1969-1919802	19690416
LA 1919781	C3	1970-0206	GB 1969-17899	19690416
GR 1224901	A	1971-0371	GB 1969-17899	19690416
SE 73137	A	1969-0223	SE 1969-132724	19690402
SE 731549	A	1969-0115	SE 1969-731549	19690415
CA 5152741	A	1971-1115	CA 1969-515274	19690415
CA 5152742	A	1971-1115	CA 1969-515275	19690415
CA 518276	A	1972-0131	CA 1969-518276	19690415
CA 518277	A	1972-0131	CA 1969-518277	19690415
CA 542197	A	1973-1115	CA 1973-11556	19690415
SE 744203	B	1974-0406	SE 1969-5290	19690415
SE 744204	B	1974-0406	SE 1969-5291	19690415
CS 160101	NO	1970-0228	CS 1969-2678	19690415
CS 160105	NO	1970-0228	CS 1969-4769	19690415
CS 160120	NO	1970-0228	CS 1969-8229	19690415
CS 160123	NO	1970-0228	CS 1969-8227	19690415
CS 160124	NO	1970-0228	CS 1969-8226	19690415
US 6903346	A	1969-0220	US 1969-690346	19690416
FR 2007446	A	1969-0223	FR 1969-11879	19690416
AT 297496	B	1970-0210	AT 1969-11444	19690416
AT 298373	B	1970-0210	AT 1969-11445	19690416
AT 298375	B	1970-0210	AT 1969-11446	19690416
SE 419027	A3	1974-0305	SE 1969-1324701	19690416
ZP 4901779	B	1974-0407	ZP 1969-294071	19690416
ZP 5100142	B	1976-0225	ZP 1973-721441	19730426
ZP 5100143	B	1976-0225	ZP 1973-721442	19730426
ZP 5100144	B	1976-0225	ZP 1973-721443	19730426
US 3960692	A	1976-0601	US 1973-374762	19730426

LA ANSWER IS OF 15 CARBON COPYRIGHT 2009 ACS ON STN (Continued)

US 1970-35007

GI For diagrams, see printed CA issue.

AS The preparation of novel thioethes (I, III) and carbon derive (III, IV) with antiinflammatory, hypcholesterolemic, antipyretic, and antipyretic properties is described. Thus, a mixture of 2 g 1 (0 = CHCO₂) (prepared from I (0 = CHO), m. p. 82-1°, via I (0 = CHCO₂), n. d. 125-127°, and I (0 = CHCO₂), m. p. 100-101°, via II (0 = CHCO₂)) and 1.5 g concentrated H2BO4 was refluxed 17 hr, to give I (0 = CHCO₂), a. d. 64-8° (perchlorate ether). Similarly were prepared the following derivs. type of compoundand n.p., given: II, CO₂H, 64.5-5.1°; III, CO₂H, 105-7°;II, 1,1-dimethyl-1,2-CH(=O)CO₂H, 110-111°; III, 1,1-dimethyl-1,2-CH(=O)CO₂H, 74-5°; IV, 1,1-dimethyl-1,2-CH(=O)CO₂H, 105-106°;IV, 1,1-dimethyl-1,2-CH(=O)CO₂H, 105-106°; IV, 1,1-dimethyl-1,2-CH(=O)CO₂H, 105-106°; IV, 1,1-dimethyl-1,